Experimental report

08/09/2022

Proposal: **EASY-857** **Council:** 10/2020

Title: Crystal structure of rare-earth Dy3B2C3O12 garnets

Research area: Physics

This proposal is a new proposal

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Experimental team:

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Samples: Dy3Sc2Ga3O12 and Dy3In2Ga3O12

Instrument	Requested days	Allocated days	From	To
D2B	4	4	16/05/2021	17/05/2021

Abstract:

The magnetic ground states of two rare-earth garnets Dy3Sc2Ga3O12 and Dy3In2Ga3O12 have been studied by neutron powder diffraction (D1B@ILL) during the last ILL cycle. Both compounds order with a k=0 multi-axis antiferromagnetic structure.

We wish therefore to carry out high-resolution neutron powder diffraction (HRNPD) at RT on those two compositions, to position oxygen atoms precisely and to evaluate the distribution of atoms on the different sites, and in particular the possible substitution of Dy3+ on the B site, occupied by Sc or In.

Analysis of the HRNPD data will lead to a proper modelling of the crystal structure for both garnets, this being a prerequisite to estimate the value of the ordered Dy3+ moment accurately in the ordered magnetic state. Moreover, it will allow us also to construct a reasonable point charge starting model before fitting CEF excitations (beamtime has been allocated on Panther@ILL to study CEF excitations in June 2021).

Crystal structure of rare-earth $Dy_3B_2C_3O_{12}$ garnets

The hyperkagome network is made of corner sharing triangles, and can be seen as a 3D analog of the planar kagome networks (Figure 1) [1,2]. Interestingly, rare-earth garnets $RE_3B_2C_3O_{12}$ (B and C chosen non magnetic) provide a realization of the hyperkagome lattice. They crystallize in a cubic structure (SG : *Ia*-3*d*), and the magnetic RE^{3+} ions occupy the sites of two nesting hyperkagome networks. They contain three distinct sites with different oxygen coordination: a dodecahedral site, occupied by RE, as well as an octahedral and a tetrahedral site, occupied by B and C, respectively (Figure 1).

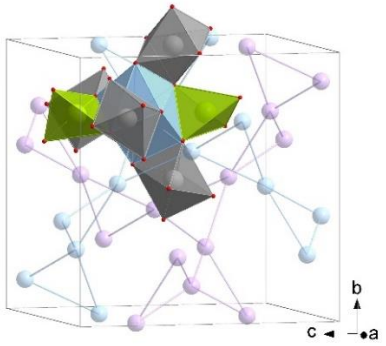

Figure 1: Dodecahedral (A site, blue), octahedral (B site, grey) and tetrahedral (C site, green) coordination in garnet $RE_3B_2C_3O_{12}$. Some atoms have been omitted for clarity. The two RE hyperkagome networks are also shown in light pink and blue).

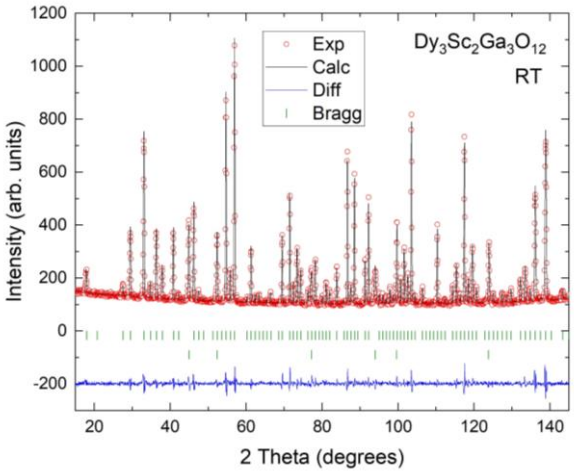

Figure 2: Rietveld refinement of the powder neutron diffractogram of $Dy_3Sc_2Ga_3O_{12}$ garnet at RT (R_{Bragg} = 3 %).

In these compounds, magnetic properties can vary radically with small changes in the crystal structure, such as those induced by chemical pressure, i.e., by changing the size of the non-magnetic cations in the lattice. Such changes will also affect the RE environment, thus modifying the crystal electric field and therefore the single-ion anisotropy of the magnetic RE^{3+}.

We have really recently studied such chemical pressure effects in two Dy garnets, namely $Dy_3Al_5O_{12}$ and $Dy_3Ga_5O_{12}$ [3]. Our goal was to extend our findings to two other garnets, $Dy_3Sc_2Ga_3O_{12}$, and $Dy_3In_2Ga_3O_{12}$.

To this end, high-resolution neutron powder diffraction was carried out at RT on D2B on those two compositions, to position oxygen atoms precisely and to evaluate the distribution of atoms on the different sites. Although no substitution on the Dy^{3+} site was observed, significant substitution (around 15%) of Ga on the In or Sc site was refined for both garnets (Figure 2).

The magnetic ground states of those two garnets have also been studied by neutron powder diffraction (D1B@ILL) during the last ILL cycle. The crystal structure data obtained on D2B was used first to extract the Dy^{3+} ordered magnetic moment, and second to build a proper point charge model, so as to determine crystal field parameters properly.

References

[1] R. Cava R et al., Introduction to Frustrated Magnetism: Materials, Experiments, Theory (Springer Berlin Heidelberg) pp 131–54 (2011)

[2] J. Hopkinson et al., Phys. Rev. Lett. 99, 037201 (2007)

[3] I. Kibalin et al., Phys. Rev. Research 2, 033509 (2020)